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A Note on Boundary Conditions for Quantum Hydrodynamic Equations

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Abstract—The asymptotic behavior of the thermal equilibrium state of a bipolar quantum hydrodynamic model is considered. The quantum limit $L \to 0$, L denoting a characteristic device length, is carried out rigorously. It shows that the classical assumption of charge neutrality at the boundary becomes invalid for ultra small semiconductor devices, whereas the assumption of vanishing boundary quantum effects will be confirmed. Furthermore, numerical simulations are presented, which give insight in the quantitative behavior.

Keywords—Quantum hydrodynamics, Thermal equilibrium, Boundary conditions for quantum models, Quantum limit.

1. INTRODUCTION

During the last years Quantum Hydrodynamic models (QHDs) gained considerable attention because of their capability to simulate quantum semiconductor devices numerically very efficiently. QHD's were able to reproduce phenomena based on quantum effects such as tunneling of carriers through potential barriers [1].

The QHD has the advantage of dealing with macroscopic fluid-type quantities, like the particle densities n and p of electrons and holes, respectively. While there is the possibility to derive the QHD equations from a nonlinear single state Schrödinger equation [2], there is to the author's knowledge no rigorous derivation of boundary conditions for the QHD from microscopic quantum models, especially not for the nonequilibrium problem. Instead, one uses boundary conditions, which proved to be valid for classical semiconductor models [3].

We only assume that the particle densities and the potential take on their equilibrium values at the boundary. For the investigation of the thermal equilibrium state we employ the variational approach of Unterreiter [4]. Due to the assumption of total charge neutrality of the device, there is no need for prescribing boundary conditions.

The thermal equilibrium state of a bipolar, isothermic quantum fluid confined to a bounded smooth domain $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, is entirely described by the particle densities n and p, where

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the pair (n, p) is a minimizer of the energy functional [4]

$$\mathcal{E}(n,p) = \frac{\hbar^2}{6\,m_n}\int |\nabla\sqrt{n}|^2 + \frac{\hbar^2}{6\,m_p}\int |\nabla\sqrt{p}|^2 \\ + k_B T \int H(n) + k_B T \int H(p) + \frac{\epsilon}{2}\int |\nabla V\,[n-p-C]|^2 .$$

Here, $V := V[n-p-C]$ denotes the self-consistent electrostatic potential, which is a solution of the Poisson equation $-\epsilon\Delta V = q\,(n-p-C)$. The function $H(t)$ is a primitive of the enthalpy function $h(t) = \log t$, which corresponds to the isothermal pressure function $p(t) = t$ by the relation $p'(t) = t\,h'(t)$. For later use we define $H_{\min} = \min\{H(t) : t > 0\}$. The physical constants and parameters are the reduced Planck constant $\hbar$, the effective masses m_n, and m_p of electrons and holes, respectively, the elementary charge q, the Boltzmann constant k_B, the permittivity ϵ, the temperature T, and the distribution of charged background ions $C = C^+ - C^-$, with C^+, $C^- > 0$, and $C \in L^\infty(\Omega)$. We define

$$N := \int C^+, \qquad P := \int C^-,$$

and seek the minimizer of $\mathcal{E}$ in the set

$$M = \left\{(n,p) \in \left[L^1(\Omega)\right]^2 : n,p \geq 0,\ \sqrt{n}, \sqrt{p} \in H^1(\Omega),\ \int n = N,\ \int p = P\right\},$$

where the constraints on the integrals over n and p correspond to the assumption of total charge neutrality of the device in thermal equilibrium. They insure the existence of exactly one potential V satisfying $\int V = 0$.

Let L be a characteristic length of the device under consideration. A rigorous analysis of the limit $L \to 0$ will show that the classical assumption of charge neutrality at the boundary [5],

$$n - p - C = 0, \qquad \text{on } \partial\Omega,$$

becomes invalid for ultra small devices, where quantum effects play a predominant role. On the other hand, we will confirm the heuristic assumption of vanishing quantum effects:

$$\frac{\Delta\sqrt{n}}{\sqrt{n}} = \frac{\Delta\sqrt{p}}{\sqrt{p}} = 0, \qquad \text{on } \partial\Omega.$$

Despite this analytic investigations, we will present numerical examples, which give evidence that also the charge neutrality at the boundary is good approximation as long as the length of the device under consideration is not too small.

The paper is organized as follows. In Section 2, we introduce a problem specific scaling, which enlightens the dependence on L. The quantum limit $L \to 0$ is investigated in Section 3 and numerical studies of a diode are presented in Section 4.

2. SCALING

For the subsequent analysis it is convenient to introduce the following scaling, where the new dimensionless variables are marked by a tilde:

$$x \to L\,\tilde{x}, \qquad n \to C_m\,\tilde{n}, \qquad p \to C_m\,\tilde{p},$$
$$V \to U_T\,\tilde{V}, \qquad C \to C_m\,\tilde{C}.$$

Here, L denotes a characteristic device length, C_m the maximal density of charged background ions, and $U_T = k_B T/q$ the thermal voltage. Introducing $\mathcal{E}_L = L^{2-d}\tilde{\mathcal{E}}$ and defining the constants

$$c_n^2 = \frac{\hbar^2}{6\,k_B\,T\,m_n}, \qquad c_p^2 = \frac{\hbar^2}{6\,k_B\,T\,m_p}, \qquad c_V^2 = \frac{\epsilon\,k_B\,T}{q\,C_m}$$

yields the scaled functional

$$\begin{aligned}\mathcal{E}_L(n,p) &= c_n^2 \int |\nabla\sqrt{n}|^2 + c_p^2 \int |\nabla\sqrt{p}|^2 \\ &\quad + L^2 \int H(n) + L^2 \int H(p) + \frac{c_V^2}{2} \int |\nabla V_L\,[n-p-C]|^2,\end{aligned} \tag{1}$$

where we omitted the tilde for notational convenience. The potential V_L is the solution of $-c_V^2 \Delta V_L = L^2(n-p-C)$, subject to $\int V_L = 0$. Note that $\mathcal{E}_L$ has the same minimizer as $\mathcal{E}$. The following existence and uniqueness result is available [4].

THEOREM 1. *$\mathcal{E}_L$ possesses a unique minimizer $(n_L, p_L) \in M$ such that there exists a constant $K_L > 0$ with $1/K_L \le n_L, p_L \le K_L$. Furthermore, there exist Lagrange-multipliers $\alpha_{1L}, \alpha_{2L} \in \mathbb{R}$ such that n_L, p_L, V_L fulfill the Euler-Lagrange-equations*

$$-c_n^2 \Delta\sqrt{n_L} + \sqrt{n_L}\left(L^2 \log(n_L) + V_L + \alpha_{1L}\right) = 0, \tag{2a}$$

$$-c_p^2 \Delta\sqrt{p_L} + \sqrt{p_L}\left(L^2 \log(p_L) - V_L + \alpha_{2L}\right) = 0, \tag{2b}$$

$$-c_V^2 \Delta V_L - L^2\,(n_L - p_L - C) = 0. \tag{2c}$$

Additionally, n_L, p_L, V_L satisfy homogeneous Neumann boundary conditions.

3. THE QUANTUM LIMIT $L \to 0$

Letting L tend formally to zero in (1) yields the functional

$$\mathcal{E}_0(n,p) = c_n^2 \int |\nabla\sqrt{n}|^2 + c_p^2 \int |\nabla\sqrt{p}|^2.$$

We assume without loss of generality that $\mu_d(\tilde{\Omega}) = 1$, where μ_d denotes the d-dimensional Lebesgue measure. One easily verifies that $(n_0, p_0) := (N, P) \in M$ is the unique minimizer of $\mathcal{E}_0$ in M, since there are no other constants in M.

We establish weak convergence of the densities by deriving *a priori* estimates independent of L; then we will use properties of the functional to get even strong convergence.

THEOREM 2. *Let (n_L, p_L) be the unique minimizer of $\mathcal{E}_L$ with corresponding potential V_L. Then, for $L \to 0$*

$$\sqrt{n_L} \to \sqrt{N}, \quad \sqrt{p_L} \to \sqrt{P}, \quad V_L\,[n_L - p_L - C] \to 0, \qquad \textit{strongly in } H^1(\Omega).$$

PROOF. Since (n_L, p_L) is the minimizer of $\mathcal{E}_L$ in M, we have

$$\mathcal{E}_L\,(n_L, p_L) \le \mathcal{E}_L(N, P).$$

This implies

$$\begin{aligned}0 &\le c_n^2 \int |\nabla\sqrt{n_L}|^2 + c_p^2 \int |\nabla\sqrt{p_L}|^2 \\ &\quad + L^2 \int \left(H\,(n_L) + H\,(p_L) - 2\,H_{\min}\right) + \frac{c_V^2}{2} \int |\nabla V_L[n_L - p_L - C]|^2 \\ &\le L^2 \int \left(H(N) + H(P) - 2\,H_{\min}\right) + \frac{c_V^2}{2} \int |\nabla V_L[N - P - C]|^2 \\ &\xrightarrow{L \to 0} 0.\end{aligned}$$

Since all summands are nonnegative, we get for $L \to 0$

$$\int |\nabla\sqrt{n_L}|^2 \to 0, \qquad \int |\nabla\sqrt{p_L}|^2 \to 0, \qquad \int |\nabla V_L[n_L - p_L - C]|^2 \to 0.$$

From Poincaré's inequality we can immediately deduce that $V_L[n_L - p_L - C] \to 0$, strongly in $H^1(\Omega)$. Furthermore, we have for $L > 0$ and some positive constant c

$$\|\sqrt{n_L}\|_{H^1}^2 = N + \int |\nabla\sqrt{n_L}|^2 \le c, \qquad \|\sqrt{p_L}\|_{H^1}^2 = P + \int |\nabla\sqrt{p_L}|^2 \le c.$$

Thus, we might extract a subsequence such that $\sqrt{n_L} \rightharpoonup \rho_*$ and $\sqrt{p_L} \rightharpoonup \sigma_*$ weakly in $H^1(\Omega)$. The embedding $H^1(\Omega) \hookrightarrow L^4(\Omega)$ is compact up to three space dimensions, such that $n_L \to \rho_*^2$ and $p_L \to \sigma_*^2$ strongly in $L^2(\Omega)$. Employing the weak lower semicontinuity of $\mathcal{E}_0$ we get

$$\begin{aligned}\mathcal{E}_0\left(\rho_*^2, \sigma_*^2\right) &\le \liminf_{L\to 0} \mathcal{E}_0\left(n_L, p_L\right) \\ &\le \liminf_{L\to 0} \left(\mathcal{E}_L\left(n_L, p_L\right) - 2\,L^2 H_{\min}\right) \\ &\le \liminf_{L\to 0} \mathcal{E}_L(N, P) = \mathcal{E}_0(N, P).\end{aligned}$$

Hence, the uniqueness of the minimizer implies $\rho_*^2 = N$ and $\sigma_*^2 = P$, from which the assertion follows. ∎

Theorem 2 can be interpreted as follows. Assuming that either $C^+ \not\equiv$ const or $C^- \not\equiv$ const, we have $N - P - C|_{\partial\Omega} \neq 0$, such that the classical charge neutrality assumption $(n - p - C)|_{\partial\Omega} = 0$ cannot be fulfilled for ultra small devices. But this is only an asymptotic result and we present in the next section numerical simulations, which will give some quantitative ideas.

Next, we investigate the assumption of vanishing boundary quantum effects, which will be confirmed by the following result.

THEOREM 3. *Let the same notations as in the previous theorem hold. Then,*

$$\frac{\Delta\sqrt{n_L}}{\sqrt{n_L}} \to 0, \quad \frac{\Delta\sqrt{p_L}}{\sqrt{p_L}} \to 0, \qquad \textit{strongly in } L^2(\Omega).$$

PROOF. We only consider the sequence $(\Delta\sqrt{n_L}/\sqrt{n_L})$, since for $(\Delta\sqrt{p_L}/\sqrt{p_L})$, one may use the same arguments. Following the proof of Theorem 2, we deduce

$$\frac{1}{L^2}\int |\nabla\sqrt{n_L}|^2 \le c, \quad \int H(n_L) \le c,$$

for some positive constant c independent of L. Multiplication of (2a) with $\sqrt{n_L}/L^2$ and integration gives

$$N\int \frac{\alpha_{1L}}{L^2} = \frac{c_n^2}{L^2}\int |\nabla\sqrt{n_L}|^2 + \int \left(H\left(n_L\right) - H_{\min}\right) + \frac{1}{L^2}\int n_L V_L - \int \left(N - H_{\min}\right),$$

from which $\alpha_{1L} = O(L^2)$ for $L \to 0$ follows due to

$$\frac{1}{L^2}\int n_L\, V_L \le c\,\|n_L\|_{L^2}\,\|n_L - p_L - C\|_{L^2}\,.$$

These bounds can be used to derive the existence of a uniform bound $K > 0$ such that $1/K \le n_L \le K$ holds for all $L > 0$ (cf. [4,6]). Taking the square of (2a) and integration yields

$$c_n^2\int \left|\frac{\Delta\sqrt{n_L}}{\sqrt{n_L}}\right|^2 \le 4\left(L^2\int |\log(K)|^2 + \int |V_L|^2 + \int \alpha_{1L}^2\right) \underset{L\to 0}{\longrightarrow} 0.$$ ∎

Thus, the quantum Bohm potentials $\Delta\sqrt{n_L}/\sqrt{n_L}$ and $\Delta\sqrt{p_L}/\sqrt{p_L}$ converge to zero almost everywhere.

REMARK 1. The Lagrange-multipliers α_{1L} and α_{2L} can be interpreted as the equilibrium values of the corresponding quantum quasi Fermi levels [4], which accordingly also vanish asymptotically.

4. NUMERICAL STUDIES

We consider a one-dimensional n^+-n-n^+-diode fabricated of GaAs with maximal doping density $C_m = 10^{24}\text{m}^{-3}$ at temperature $T = 77\,\text{K}$. For the values of the physical parameters, we refer to [5]. The equilibrium solutions for different lengths L (= 20, 100, 200 nm) of the device were computed by a gradient projection method (cf. [7]).

Figure 1 shows the computed electron densities for various lengths of the device and also the doping profile for reference. Clearly, one verifies the convergence predicted in Theorem 2. In Table 1, we present some values of the relevant quantities at the left boundary point of the device, which give evidence that the results hold only asymptotically. Charge neutrality at the boundary is still valid for ultra small devices (100 nm), whereas there seems to be a range in which the assumption of vanishing quantum effects does not hold. Also the equilibrium values of the potential and the quantum quasi Fermi level cannot be neglected. Note that they almost coincide if the device is sufficiently large.

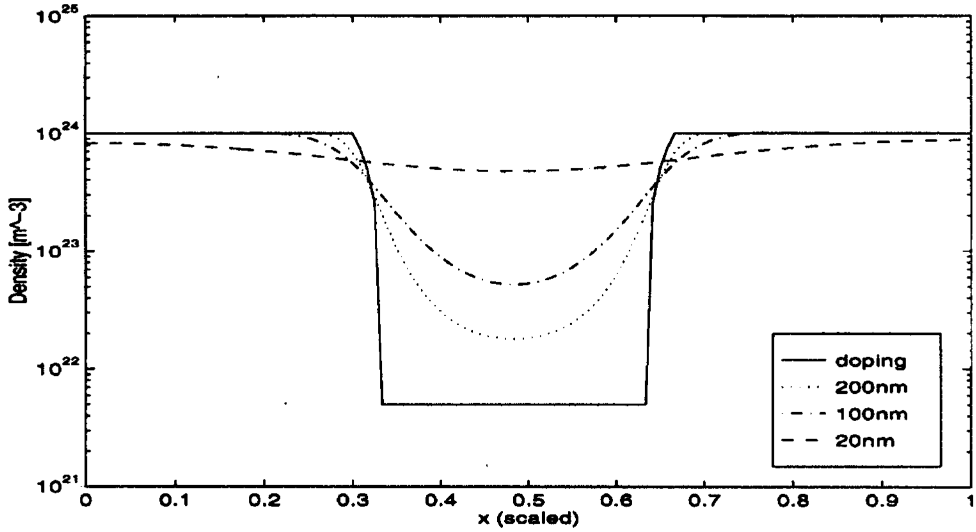

Figure 1. Equilibrium densities.

Table 1. Numerical results.

L	$n(0)$	$\frac{\Delta\sqrt{n(0)}}{\sqrt{n(0)}}$	$V(0)$	α
20 nm	0.83	−4.3	−0.6	−0.46
100 nm	0.999	−0.03	−0.868	−0.87
200 nm	0.999	0.07	−1.113	−1.115

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